Effects of dimerization and interchain one-particle hopping in a weakly coupled dimerized chain system at quarter filling

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Abstract
Effects of the intrachain dimerization and the interchain one-particle hopping, t_b, in a quasi-one-dimensional dimerized chain system at quarter filling have been studied, based on the perturbative renormalization group (PRG) approach. Based on the results, we discuss difference in the low-energy properties between TMTTF and TMTSF compounds.
Keywords: Many-body and quasiparticle theories, Magnetic phase transitions, Organic conductors based on radical cation and/or anion salts

1. INTRODUCTION

Quasi-one-dimensional (Q1D) organic conductors $(TMTTF)_2X$ and $(TMTSF)_2X$ (X=Br, PF_6,...) have in common the 2:1 stoichiometry, which makes the band quarter-filled, and the dimerized one-particle hopping integrals, t_{a1} and t_{a2}, along the conducting stack [1]. The ratios of the one-particle hopping integrals along the high and intermediate directions, t_a and t_b, are approximately $t_b/t_a \sim 0.04$ and 0.1 for TMTTF and TMTSF compounds, respectively.

In spite of the similarity in electronic structure, their low temperature transport and magnetic properties are essentially different. At ambient pressure, $(TMTTF)_2Br$ is semiconducting with a shallow minimum in resistivity and undergoes a phase transition to a commensurate spin-density wave (CSDW) phase [2]. In contrast, $(TMTSF)_2PF_6$ shows metal-like behavior down to a phase transition to an incommensurate SDW (ICSDW) [3]. Optical reflectivity spectra above the phase transition temperature indicate the one-particle propagation is *confined* in a single chain at any temperature for $(TMTTF)_2Br$, but it is *deconfined* at low temperatures for $(TMTSF)_2PF_6$ [4].

As was stressed by Emery *et al.* [5], important difference between TMTTF and TMTSF compounds is the degree of dimerization, $\Delta = (t_{a1} - t_{a2})/(t_{a1} + t_{a2})$, evaluated as 0.2 and 0.05, respectively [6]. In terms of g-ology [7], the intrachain backward, forward and $2k_F$-umklapp scattering strengths in a dimerized chain at quarter filling are given by $\pi v_F g_1 = U/2 - V$, $\pi v_F g_2 = U/2 + V$, $\pi v_F g_3 = (U/2 - V)\, 2\Delta/(1 + \Delta^2)$ [8], where g_i are dimensionless scatering strengths with v_F being the Fermi velocity and U, V denoting the on-site and the nearest neighbor Coulomb repulsions, respectively. Therefore stronger Δ causes stronger g_3. Recently, based on the perturbative renormalization group (PRG) approach [9], we discussed the effects of the umklapp scattering in a weakly-coupled *half-filled* chain system [10]. We here extend the work to the case of a weakly coupled dimerized chain system at quarter filling where a finite dimerization causes a finite umklapp scattering strength.

2. PRG FORMULATION

We consider a 2D array of an infinite number of chains weakly coupled via interchain one-particle hopping t_b. As in Ref. [10], we treat renormalization flows of g_i by solving the 2-loop PRG equations [11]. When the initial values of g_i satisfy the condition $g_1 - 2g_2 <\mid g_3 \mid$, the umklapp process becomes relevant and the 2-loop RG equations give the non-trivial fixed point, $g_1^* = 0$ and $\mid g_3^* \mid = 2g_2^* - g_1^* = 2$. From now on, we consider only this parameter region. In the absence of the interchain coupling, the fixed point corresponds to the Mott insulator phase with short-range antiferromagnetic (AF) correlation.

The 2-loop PRG equation for t_b is given by [11,12]

$$d\ln t_b/dl = 1 - \left({g_1}^2 + {g_2}^2 - g_1 g_2 + {g_3}^2/2\right)/4, \tag{1}$$

where the scaling parameter, l, is related to the absolute temperature, T, as $l = \ln[E_0/T]$ with the high-energy bandwidth cutoff, E_0, which is of the order of the intrachain hopping integral, t_a. In the course of the renormalization, t_b attains the order of the initial bandwidth, E_0, at some crossover value of the scaling parameter, $l_{\rm cross} = \ln[E_0/T_{\rm cross}]$, qualitatively defined by $t_b(l_{\rm cross}) = E_0$.

In the paramter region considered here, the most dominant interchain two-particle process *dynamically generated* in the course of the scaling [9] is the interchain $2k_F$ spin-spin interaction. The corresponding interaction Hamiltonian is written as

$$\mathcal{H}_\perp^{\rm int} = \frac{\pi v_F}{4} \sum_{\vec{q}} \left[J(q_b) \vec{S}_{\vec{q}}^* \cdot \vec{S}_{\vec{q}} + K(q_b)(\vec{S}_{\vec{q}}^* \cdot \vec{S}_{\vec{q}}^* + \vec{S}_{\vec{q}} \cdot \vec{S}_{\vec{q}}) \right], \tag{2}$$

where $\vec{S}_{\vec{q}}$ denotes the $2k_F$ spin density field with the momentum $\vec{q} = (2k_F, q_b)$ (q_b denotes the momentum perpendicular to the chain).

The PRG equations for the interchain spin-spin interactions are written as

$$\begin{aligned} dJ(q_b)/dl &= \frac{1}{2}\tilde{t}_b^2 \left[{g_2}^2 + 4{g_3}^2\right] \cos q_b + \frac{1}{2}\left[g_2 J(q_b) + 4 g_3 K(q_b)\right] - \frac{1}{4}\left[J(q_b)^2 + 4K(q_b)^2\right], \\ dK(q_b)/dl &= 2\tilde{t}_b^2 g_2 g_3 \cos q_b + 2\left[g_2 K(q_b) + g_3 J(q_b)\right] - J(q_b)K(q_b), \end{aligned} \tag{3}$$

where $\tilde{t}_b \equiv t_b/E_0$. Although $J(q_b) = K(q_b) = 0$ at the initial step, the third term causes divergence of them at a critical scaling parameter $l_{\rm SDW} = \ln[E_0/T_{\rm SDW}]$ defined by $J(q_b) = K(q_b) = -\infty$. The value of $l_{\rm SDW}$ becomes minimum for $q_b = \pi$ corresponding to a 2D commensurate SDW phase(i.e., 2D AF phase). From now on, we fix $q_b = \pi$ and replace $T_{\rm SDW}$ with the Neel temperature, T_N.

3. PHASE DIAGRAM

To see which of $T_{\rm cross}$ and T_N is larger, we solve the coupled scaling equations (1), (3) and (3). We treat the RG flows of g_i through the 2-loop PRG equations. As to the initial conditions for the intrachain Coulomb repulsions, we use $U = 4V = 1.6\pi v_F$.

In Fig. 1, we show a phase diagram spanned by t_{b0} (the initial value of the interchain one-particle hopping integral) and T for $\Delta = 0.2$. There exists a critical value of t_b: $t_b^* \sim 0.23E_0$. For $t_b < t_b^*$, the interchain one-particle propagation is strongly suppressed and the 2D AF phase is stabilized at T_N. For $t_b > t_b^*$, the interchain one-particle propagation develops and the system undergoes a crossover to the Fermi liquid (FL) phase. In the FL phase, the phase transition to the SDW phase due to the Fermi surface nesting is possible, where the SDW vector

is determined by the optimal nesting condition which generally leads to the ICSDW transition. In this case, the increasing t_b decreases the degree of nesting and consequently decreases the SDW transition temperature [13] and finally a superconducting transition is caused by the spin fluctuation mechanism [14].

In Fig. 2, we show how t_b^* depends on Δ. We see that a finite Δ causes a finite t_b^*. As Δ becomes weaker, the AF phase in Fig. 1 shrinks. This situation comes from the fact that the umklapp scattering becomes less important and the suppression of the interchain one-particle hopping becomes weaker with the decreasing Δ, and consequently the interchain one-particle propagation can acquire coherence even for small t_b. Provided that TMTTF and TMTSF compounds have the same strength of the intrachain interaction, $U = 4V = 1.6\pi v_F$, t_b and Δ of TMTTF and TMTSF compounds are located at the points indicated in Fig. 2. We see the point of TMTTF lies in the AF region, while the points of TMTSF lies near the boundary between the AF and the FL phase.

4. SUMMARY

Based on the PRG approach, we have studied the effects of the dimerization, Δ, and the interchain one-particle hopping integral, t_b, in the weakly coupled dimerized chain system at quarter filling. A finite dimerization causes a finite strength of the intrachain umklapp scattering and consequently the interchain one-particle propagation is strognly suppressed. Then the low-energy asymptotics of the system is determined through Δ and t_b. The present results qualitatively explain the difference in the low-energy properties between TMTTF and TMTSF compounds.

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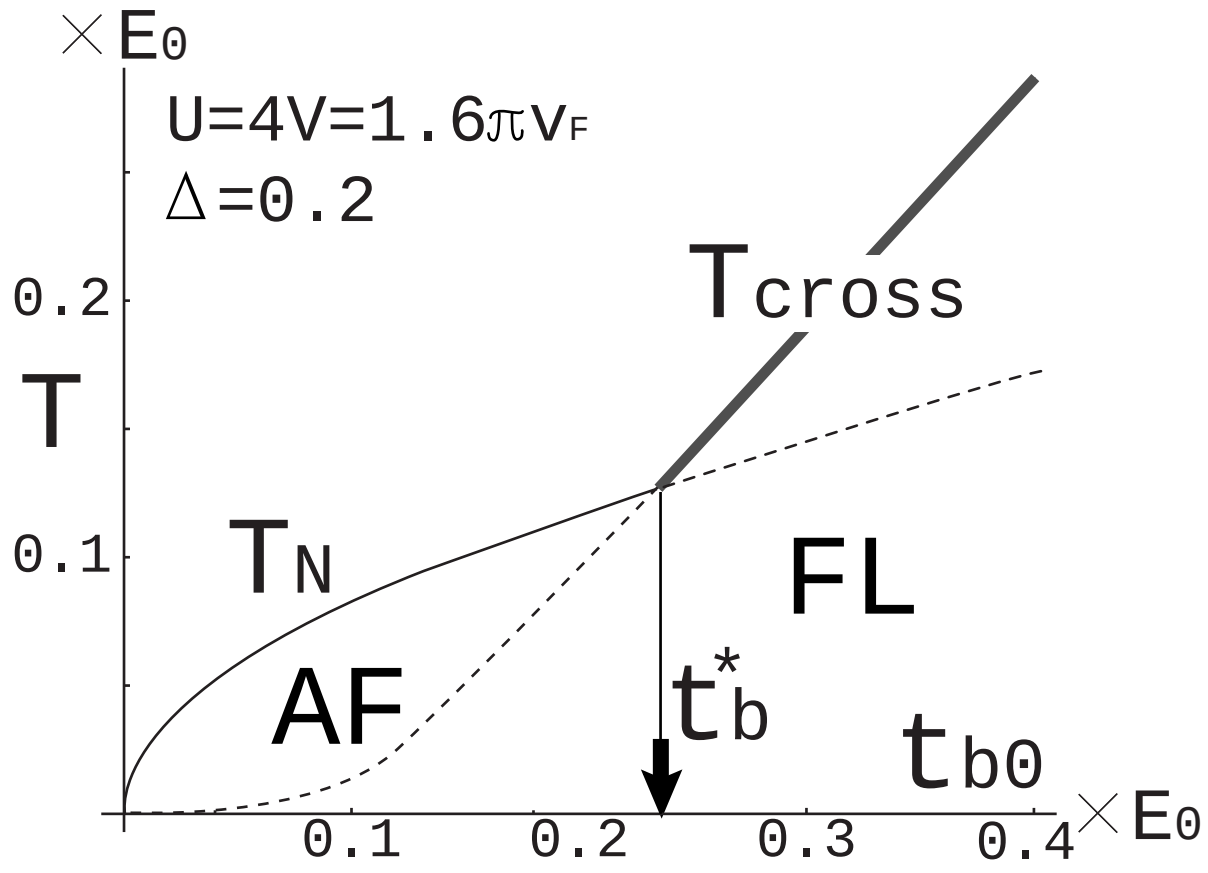
FIG. 1. Phase diagram. **AF** and **FL** are the abbreviations for the antiferromagnetic phase and the Fermi liquid phase, respectively.

FIG. 2. Dependence of t_b^* on Δ. t_b and Δ of TMTTF and TMTSF compounds are indicated.


×E0
U=4V=1.6πvF
Δ=0.2
0.2
T
0.1
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TN
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AF
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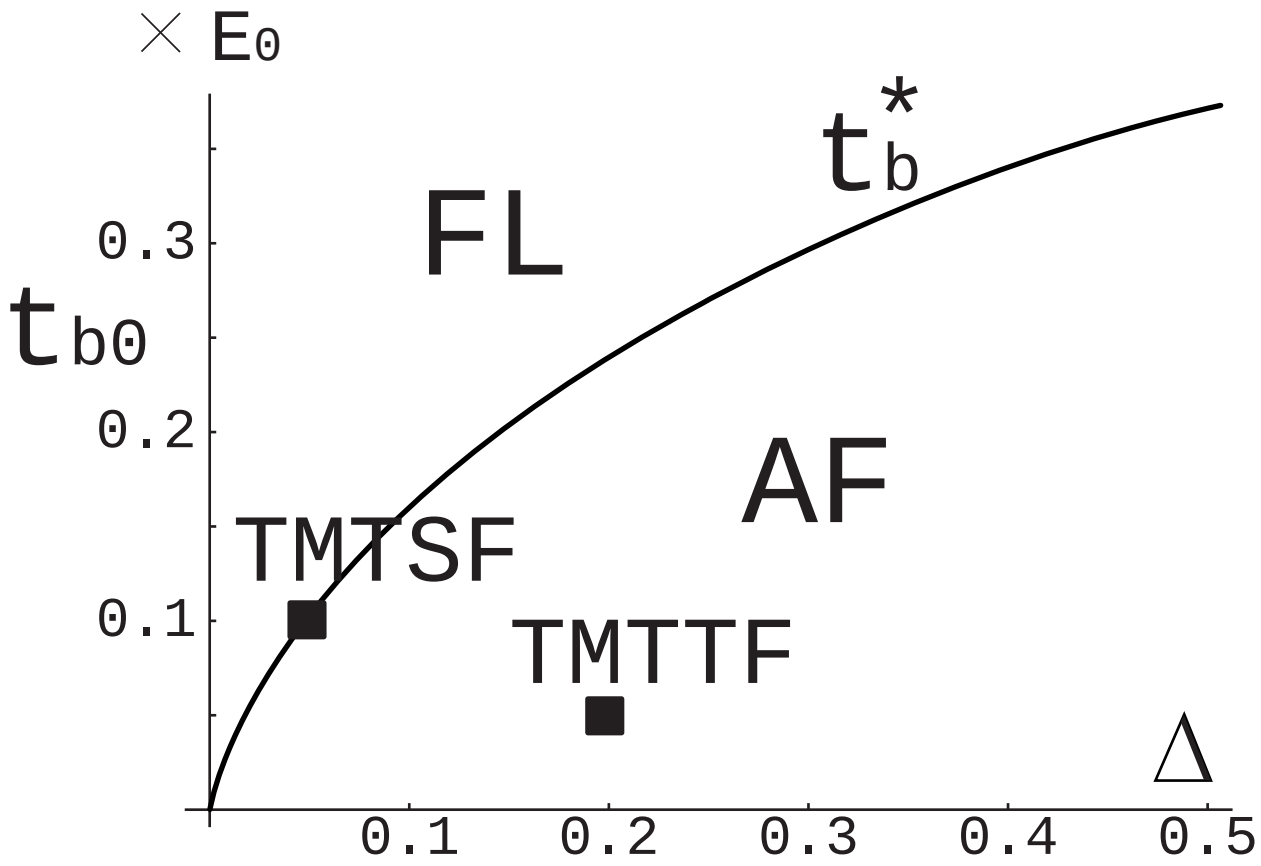
×E0


× E0
t*b
FL
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TMTSF
TMTTF
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0.3
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